

# SAFETY DATA SHEETS

According to the UN GHS revision 9

Version: 1.0  
Creation Date: July 15, 2019  
Revision Date: July 15, 2019

## SECTION 1: Identification

### 1.1 GHS Product identifier

**Product name** 4-tert-butyltoluene

### 1.2 Other means of identification

**Product number** -

**Other names** Benzene, 1-(1,1-dimethylethyl)-4-methyl-; 1-tert-butyl-4-methylbenzene

### 1.3 Recommended use of the chemical and restrictions on use

**Identified uses** Industrial and scientific research use.

**Uses advised against** no data available

### 1.4 Supplier's details

**Company** Shanghai Baishun Biotechnology Co., Ltd  
**Address** No. 26, Lane 918, Lianye Road, Zhelin Town, Fengxian District, Shanghai, 201400, China  
**Telephone** +86-21-37581181

### 1.5 Emergency phone number

**Emergency phone number** +86-21-37581181

**Service hours** Monday to Friday, 9am-5pm (Standard time zone: UTC/GMT +8 hours).

## SECTION 2: Hazard identification

### 2.1 Classification of the substance or mixture

Acute toxicity - Category 4, Oral  
Acute toxicity - Category 2, Inhalation  
Reproductive toxicity, Category 2  
Specific target organ toxicity – single exposure, Category 1  
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 2

### 2.2 GHS label elements, including precautionary statements

**Pictogram(s)**



**Signal word** Danger  
**Hazard statement(s)** H302 Harmful if swallowed

H319 Causes serious eye irritation  
H330 Fatal if inhaled  
H361 Suspected of damaging fertility or the unborn child  
H372 Causes damage to organs through prolonged or repeated exposure  
H401 Toxic to aquatic life  
H411 Toxic to aquatic life with long lasting effects

**Precautionary statement(s)**

**Prevention**

P264 Wash ... thoroughly after handling.  
P270 Do not eat, drink or smoke when using this product.  
P260 Do not breathe dust/fume/gas/mist/vapours/spray.  
P271 Use only outdoors or in a well-ventilated area.  
P284 [In case of inadequate ventilation] wear respiratory protection.  
P203 Obtain, read and follow all safety instructions before use.  
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...

**Response**

P273 Avoid release to the environment.  
P301+P317 IF SWALLOWED: Get medical help.  
P330 Rinse mouth.  
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.  
P316 Get emergency medical help immediately.  
P320 Specific treatment is urgent (see ... on this label).  
P318 IF exposed or concerned, get medical advice.  
P308+P316 IF exposed or concerned: Get emergency medical help immediately.  
P321 Specific treatment (see ... on this label).  
P391 Collect spillage.

**Storage**

P403+P233 Store in a well-ventilated place. Keep container tightly closed.

**Disposal**

P405 Store locked up.  
P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

## 2.3 Other hazards which do not result in classification

no data available

---

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number	Concentration
4-tert-butyltoluene	4-tert-butyltoluene	98-51-1	202-675-9	100%

---

## SECTION 4: First-aid measures

### 4.1 Description of necessary first-aid measures

**If inhaled**

Fresh air, rest. Half-upright position. Refer immediately for medical attention.

**Following skin contact**

Rinse and then wash skin with water and soap.

**Following eye contact**

Rinse with plenty of water for several minutes (remove contact lenses if easily possible).

**Following ingestion**

Rinse mouth. Give one or two glasses of water to drink. Refer for medical attention .

## **4.2 Most important symptoms/effects, acute and delayed**

Exposure Routes: inhalation, ingestion, skin and/or eye contact Symptoms: Irritation eyes, skin; dry nose, throat; headache; low blood pressure, tachycardia, abnormalities cardiovascular system stress; central nervous system, hematopoietic depression; metallic taste; liver, kidney injury Target Organs: Eyes, skin, respiratory system, cardiovascular system, central nervous system, bone marrow, liver, kidneys (NIOSH, 2016)

## **4.3 Indication of immediate medical attention and special treatment needed, if necessary**

Flush eyes with water. Wash off contaminated areas of body with soap and water. Gastric lavage (stomach wash), if swallowed, followed by saline catharsis.

---

## **SECTION 5: Fire-fighting measures**

### **5.1 Suitable extinguishing media**

Fires involving this compound should be controlled with a dry chemical, carbon dioxide or halon extinguisher. (NTP, 1992)

### **5.2 Specific hazards arising from the chemical**

This chemical is combustible. (NTP, 1992)

### **5.3 Special protective actions for fire-fighters**

Use water spray, alcohol-resistant foam, dry powder, carbon dioxide.

---

## **SECTION 6: Accidental release measures**

### **6.1 Personal precautions, protective equipment and emergency procedures**

Personal protection: self-contained breathing apparatus. Do NOT let this chemical enter the environment. Ventilation. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

### **6.2 Environmental precautions**

Personal protection: self-contained breathing apparatus. Do NOT let this chemical enter the environment. Ventilation. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

### **6.3 Methods and materials for containment and cleaning up**

Absorb on paper. Evaporate on a glass or an iron dish in hood. Burn the paper.

---

## **SECTION 7: Handling and storage**

### **7.1 Precautions for safe handling**

NO open flames. Above 63°C use a closed system and ventilation. Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

### **7.2 Conditions for safe storage, including any incompatibilities**

Separated from food and feedstuffs and strong oxidants. Well closed. Keep in a well-ventilated room. Store in an area without drain or sewer access. Provision to contain effluent from fire extinguishing.

---

## **SECTION 8: Exposure controls/personal protection**

### **8.1 Control parameters**

Occupational Exposure limit values

TLV: 1 ppm as TWA

**Biological limit values**

no data available

## 8.2 Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

## 8.3 Individual protection measures, such as personal protective equipment (PPE)

**Eye/face protection**

Wear safety spectacles or eye protection in combination with breathing protection.

**Skin protection**

Protective gloves.

**Respiratory protection**

Use ventilation, local exhaust or breathing protection.

**Thermal hazards**

no data available

---

## SECTION 9: Physical and chemical properties and safety characteristics

<b>Physical state</b>	Liquid.
<b>Colour</b>	Clear, colourless.
<b>Odour</b>	DISTINCT AROMATIC ODOR
<b>Melting point/freezing point</b>	-52 °C.
<b>Boiling point or initial boiling point and boiling range</b>	193 °C. Atm. press.:1 013 hPa.
<b>Flammability</b>	Class IIIA Combustible Liquid: Fl.P. at or above 140°F and below 200°F.
<b>Lower and upper explosion limit/flammability limit</b>	no data available
<b>Flash point</b>	58.3 °C. Atm. press.:1 013.25 hPa.
<b>Auto-ignition temperature</b>	510 °C. Atm. press.:1 013.25 hPa.
<b>Decomposition temperature</b>	no data available
<b>pH</b>	no data available
<b>Kinematic viscosity</b>	dynamic viscosity (in mPa s) = 1.677. Temperature:0.0°C.
<b>Solubility</b>	less than 1 mg/mL at 63° F (NTP, 1992)
<b>Partition coefficient n-octanol/water</b>	log Pow = 4.4.
<b>Vapour pressure</b>	1.3 hPa. Temperature:30 °C.
<b>Density and/or relative density</b>	0.86 g/cm³. Temperature:20 °C.
<b>Relative vapour density</b>	4.62 (AIR= 1)
<b>Particle characteristics</b>	no data available

---

## SECTION 10: Stability and reactivity

### 10.1 Reactivity

Decomposes on burning. This produces toxic fumes. Reacts with strong oxidants. This generates fire and explosion hazard.

## 10.2 Chemical stability

no data available

## 10.3 Possibility of hazardous reactions

Flammable. Moderately dangerous fire risk. As a result of flow, agitation, etc., electrostatic charges can be generated. P-TERT-BUTYL TOLUENE may react with oxidizing materials. (NTP, 1992)

## 10.4 Conditions to avoid

no data available

## 10.5 Incompatible materials

Oxidizers.

## 10.6 Hazardous decomposition products

When heated to decomposition it emits acrid smoke and irritating fumes.

---

# SECTION 11: Toxicological information

### Acute toxicity

- Oral: LD50 - rat (male) - ca. 1 550 mg/kg bw. Remarks: Original value: LD50 = 1.8 +/- 0.14 ml/kg bw.
- Inhalation: LC50 - rat (female) - ca. 1.5 mg/L air.
- Dermal: LD50 - rabbit - ca. 16 880 mg/kg bw.

### Skin corrosion/irritation

no data available

### Serious eye damage/irritation

no data available

### Respiratory or skin sensitization

no data available

### Germ cell mutagenicity

no data available

### Carcinogenicity

no data available

### Reproductive toxicity

no data available

### STOT-single exposure

The substance is irritating to the eyes and respiratory tract. Exposure far above the OEL could cause lowering of consciousness.

### STOT-repeated exposure

The substance may have effects on the central nervous system. This may result in tissue lesions.

### Aspiration hazard

A harmful contamination of the air can be reached rather quickly on evaporation of this substance at 20°C.

---

# SECTION 12: Ecological information

## 12.1 Toxicity

- Toxicity to fish: LC50 - Cyprinus carpio - 2 mg/L - 96 h. Remarks: Concentrations are given as arithm. means of calculated test concentrations and measured test concentrations after 24 hours.
- Toxicity to daphnia and other aquatic invertebrates: EC50 - Daphnia magna - 3.2 mg/L - 48 h.
- Toxicity to algae: EC50 - Desmodesmus subspicatus (previous name: Scenedesmus subspicatus) - > 5.6 mg/L - 72 h.
- Toxicity to microorganisms: EC0 - Pseudomonas putida - >= 1 000 mg/L - 5 h. Remarks: Respiration rate.

## 12.2 Persistence and degradability

Using a standard dilution method over a 5-day inoculation period and a seed from an effluent of a biological sanitary waste treatment plant, 4-t-butyltoluene was found to have a 2% theoretical BOD when the seed was not adapted and 6% theoretical BOD when the seed was adapted(1).

## 12.3 Bioaccumulative potential

Based upon a reported water solubility of 5.5 ppm at 25 deg C(1), the BCF for 4-t-butyltoluene can be estimated to be 236 from a recommended regression-derived equation(2, SRC). This estimated BCF indicates that some bioconcentration in aquatic organisms may occur(SRC).

## 12.4 Mobility in soil

Based upon a reported water solubility of 5.5 ppm at 25 deg C(1), the Koc for 4-t-butyltoluene can be estimated to be 1700 from a linear regression-derived equation(2, SRC). Using a structure estimation method based on molecular connectivity indexes, the Koc for 4-t-butyltoluene can be estimated to be 1900(3). These estimated Koc values indicate that 4-t-butyltoluene will have low mobility in soil(4).

## 12.5 Other adverse effects

no data available

---

# SECTION 13: Disposal considerations

## 13.1 Disposal methods

### Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

### Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

---

# SECTION 14: Transport information

## 14.1 UN Number

ADR/RID: UN2667 (For reference only, please check.)

IMDG: UN2667 (For reference only, please check.)

IATA: UN2667 (For reference only, please check.)

## 14.2 UN Proper Shipping Name

ADR/RID: BUTYLTOLUENES (For reference only, please check.)

IMDG: BUTYLTOLUENES (For reference only, please check.)

IATA: BUTYLTOLUENES (For reference only, please check.)

## 14.3 Transport hazard class(es)

ADR/RID: 6.1 (For reference

IMDG: 6.1 (For reference

IATA: 6.1 (For reference

only, please check.)

only, please check.)

only, please check.)

#### 14.4 Packing group, if applicable

ADR/RID: III (For reference only, please check.)

IMDG: III (For reference only, please check.)

IATA: III (For reference only, please check.)

#### 14.5 Environmental hazards

ADR/RID: Yes

IMDG: Yes

IATA: Yes

#### 14.6 Special precautions for user

no data available

#### 14.7 Transport in bulk according to IMO instruments

no data available

---

### SECTION 15: Regulatory information

#### 15.1 Safety, health and environmental regulations specific for the product in question

Chemical name	Common names and synonyms	CAS number	EC number
4-tert-butyltoluene	4-tert-butyltoluene	98-51-1	202-675-9
European Inventory of Existing Commercial Chemical Substances (EINECS)			Listed.
EC Inventory			Listed.
United States Toxic Substances Control Act (TSCA) Inventory			Listed.
China Catalog of Hazardous chemicals 2015			Not Listed.
New Zealand Inventory of Chemicals (NZIoC)			Listed.
Philippines Inventory of Chemicals and Chemical Substances (PICCS)			Listed.
Vietnam National Chemical Inventory			Listed.
Chinese Chemical Inventory of Existing Chemical Substances (China IECSC)			Listed.
Korea Existing Chemicals List (KECL)			Listed.

---

### SECTION 16: Other information

#### Information on revision

Creation Date July 15, 2019

Revision Date July 15, 2019

#### Abbreviations and acronyms

- CAS: Chemical Abstracts Service
- ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road
- RID: Regulation concerning the International Carriage of Dangerous Goods by Rail
- IMDG: International Maritime Dangerous Goods
- IATA: International Air Transportation Association
- TWA: Time Weighted Average
- STEL: Short term exposure limit
- LC50: Lethal Concentration 50%
- LD50: Lethal Dose 50%
- EC50: Effective Concentration 50%

#### References

- IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>
- HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

- IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>
- eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: [http://www.echemportal.org/echemportal/index?pageID=0&request\\_locale=en](http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en)
- CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>
- ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>
- ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>
- Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>
- ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

### Other Information

The odour warning when the exposure limit value is exceeded is insufficient.

**Any questions regarding this SDS, Please send your inquiry to [sds@xixisys.com](mailto:sds@xixisys.com)**

---

*Disclaimer: The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. We as supplier shall not be held liable for any damage resulting from handling or from contact with the above product.*